REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-02-

0210

1. REPORT DATE (DD-MM-YYYY)	2. REPORT DATE	3. DATES COVERED (From - To)
	Final Technical Report	7/1/95 - 6/30/01

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Process Modeling & In-Situ Sensor Feedback Based Adaptive Control of Molecular Beam Epitaxy & Ion-Assisted Reactive Etching of Advanced Semiconductor Structures	F49620-95-1-0452

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)	5d. PROJECT NUMBER
Professors A. Madhukar, I. G. Rosen, R. K. Kalia, P. Vashishta, and C. Wang	

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT NUMBER
University of Southern California Dept. of Materials Science & Engineering 3651 Watt Way, VHE 506 Los Angeles, CA 90089-0241	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
AFOSR/NE 801 North Randolph Street, Room 732 Arlington, VA 22203-1977	

11. SPONSORING/MONITORING AGENCY REPORT NUMBER

12. DISTRIBUTION AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

The view, opinion, and/or findings in this report are those of the author(s) and should not be constructed as an official Department of the Air Force position, policy, or decision, unless so designated by other documentation.

14. ABSTRACT

This document summarizes the salient features of the accomplishments made during the period July 1, 1999 - June 30, 2001, of the above-titled MURI grant. The accomplishments include: (i) design and successful experimental implementation of single input (microwave power) adaptive real-time control of CF_4/O_2 plasma etching of Si_xN_y utilizing spectroscopic ellipsometry sensor feedback; (ii) development of highly efficient, dynamic load balancing, low overhead, and scalable algorithm to carry out atomistic simulations on massively parallel computing platforms and its testing for systems up to a billion atoms; (iii) multi-resolution molecular-dynamics simulations of atomic scale stress distributions and dislocation propagation in Si/Si_3N_4 nanopixels with up to 27 million atoms; (iv) developed a reflection-high-energy electron diffraction in-situ sensor based machine condition transfer function for reproducibility of molecular beam epitaxy (MBE) growth conditions; (v) examination of MBE growth on patterned surfaces and the role of surface stress engineering to achieve spatially selective growth of quantum dots; (vi) large scale molecular dynamics simulations of bare and overlayer covered nanoscale square mesas of the Ge/Si (001) and InAs/GaAs (001) systems; (vii) evidence from the InAs on GaAs (001) simulated stress relaxation for the observed self-limiting InAs overlayer thickness on GaAs nanomesas.

15. SUBJECT TERMS

Semiconductor manufacturing, in-situ sensors, real-time etching control, spectroscopic ellipsometry, molecular beam epitaxy, focused ion beam, nanostructures, silicon nitride, gallium arsenide, molecular dynamics, stresses in device nanomesas.

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL		19b. TELEPONE NUMBER (Include area code)

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI-Std Z39-18

20020719 126

Final Technical Report

July 1, 1995 – June 30, 2001

MURI '94 Program on
Process Modeling & In-Situ Sensor Feedback Based Adaptive Control of Molecular Beam
Epitaxy and Ion-Assisted Reactive Etching of Advanced Semiconductor Structures

Contract No. F49620-95-1-0452

Submitted to

Dr. Marc Jacobs
Dr. Belinda King
Air Force Office of Scientific Research

Submitted by

Anupam Madhukar
Principal Investigator
University of Southern California
Los Angeles, CA 90889-0241

Co-PIs
P. Chen
R. K. Kalia
I. G. Rosen
P. Vashishta
C. Wang

This document summarizes the objectives and salient accomplishments of the work undertaken under the above-noted MURI program.

I. Recalling Objectives

The joint efforts of researchers at the University of Southern California and Louisiana State University were focused upon understanding the scientific underpinnings and advancing the technological development of the paradigms and methodologies for in-situ sensor based control of growth and etching processes underlying semiconductor nanostructure fabrication, accounting for the synergism between nanostructure size/shape/orientation and the surface/interface mechanical stress inhomogeneities. The flow chart below depicts the two approaches to nanostructures synthesis: (a) pixellation via post-growth patterning and etching; (b) purely growth-controlled nanostructure synthesis via growth on pre-patterned substrates.
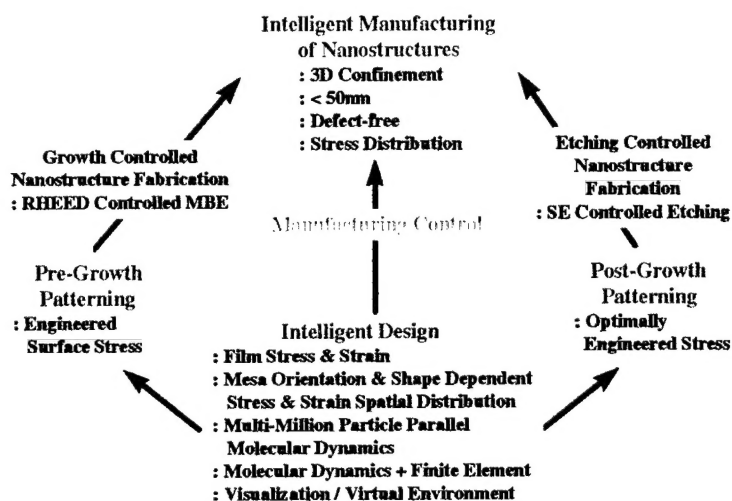
The focused objectives pertaining to these two complementary approaches were:

1. Real-time adaptive control of semiconductor/dielectric etching using Spectroscopic Ellipsometry (SE) / Optical Emission (OE) *in-situ* sensor feed-back

2. Growth-controlled nanostructure synthesis via control of molecular beam epitaxical growth on patterned and planar substrates using RHEED (reflection high-energy electron diffraction) in-situ sensor for run-to-run and machine-to-machine reproducibility of growth conditions.

3. Multimillion atom, massively parallel molecular dynamics based simulations of the spatially inhomogeneous stresses and strains in nanoscale ($\leq$ 50nm) mesas as a function of mesa orientation, shape and size.

These overall objectives involved achieving several sub-objectives that include physical modeling and simulation of selected processes and process consequences, developing empirical or phenomenological control models based upon *in-situ* sensor response, developing the algorithms and hardware to implement and test such control, developing multi-resolution (in space and time) scalable O(N) algorithms for molecular dynamics on massively parallel computing platforms, developing efficient algorithms for visualization of the massive data

generated, and developing and validating inter-atomic potential energy functions that represent the interactions in molecular dynamics simulations of semiconductor nanostructures.

II. Salient Accomplishments:

We summarize below the major accomplishments of this MURI project. These are divided into four categories relating to experiment and simulation, respectively, for each of the two approaches to nanostructure fabrication: post-growth pixellation and growth on pre-patterned mesas.

II.1 In-Situ Sensor based Real-time Adaptive Feedback Control of Semiconductor Etching

1. Developed a database and a phenomenological model of the thermal chlorine etch rate for GaAs as a function of substrate temperature and Cl_2 pressure (see publication 24).

2. Designed, simulated, tested, and successfully implemented a real time, adaptive feedback controller for thermal chlorine etching of gallium arsenide with spectroscopic ellipsometry sensing, accounting for a physically based model for the chamber valve (i.e. actuator) dynamics. The phenomenological model for the etch rate as a function of substrate temperature and Cl_2 pressure, noted under point 1 above, is utilized for adaptive control (see publications 21, 24, 37, 57, and 58).

3. Developed an artificial neural network (ANN) based approach to determining, from a limited data set, a process recipe that minimizes the sensitivity of the process output to errors in the machine sensors and actuators and implemented this methodology for the plasma enhanced chemical vapor deposition of silicon nitride dielectric films (see publications 32 and 52).

4. Carried out a 4 input variable full-factorial design-of-experiment (DoE) screening study of $CF_4/5\%O_2$ plasma etching of silicon nitride. The results indicated that microwave power and chamber pressure are the two most critical machine inputs for this plasma etch process.

5. Refined design, simulated, tested, and successfully implemented in-situ spectroscopic ellipsometry sensor based real-time, single input adaptive feedback controller for CF_4/O_2 plasma etching of silicon nitride. *Achieved a 60% improvement in machine reproducibility for the silicon nitride etch process* (see publications 30, 44, 45, and 57).

6. Designed and simulation tested two input (microwave power and chamber pressure) adaptive controller for CF_4/O_2 plasma etching of silicon nitride.

II.2. Si/Si$_x$N$_y$ Nanopixel Stress Simulations:

1. Developed and validated the first interatomic potentials for Si/SixNy interface.

2. Developed highly efficient, dynamic load balancing, low overhead, and scalable algorithm to map irregular atomistic simulations on massively parallel machines and tested it for systems containing up to 1.04 billion atoms.

3. The first multiresolution molecular-dynamics simulations containing 4, 10 and 27 million atoms were performed on parallel computers to determine atomic -level stress distributions in 25nm, 54nm and 70nm nanopixel respectively, on a 0.15 µm silicon substrate. Effects of surfaces, edges, and lattice mismatch at the silicon/silicon nitride interface on the stress distribution were investigated. Compared to the crystalline silicon nitride case, the stress in

amorphous silicon nitride is highly inhomogeneous in the plane of the interface - a triangular lattice of stress domains of size 10 nm is observed (see publications 23, 36, 38, 42, and 46).

4. Mechanical behavior of the silicon/silicon nitride interface was also studied using million atom molecular dynamics simulations. At the critical value of the strain parallel to the interface, a crack forms on the silicon nitride surface and moves toward the interface. Time evolution of dislocation emission and nature of defects was studied in atomic detail and the speed of dislocation motion was determined to be 500 m/s (see publication 47).

II.3. Growth Controlled Semiconductor Nanostructures:

1. Developed and tested the methodology and algorithm (software) for determining MBE machine condition transfer function (MCTF) based upon GaAs substrate static surface RHEED specular beam intensity data as a function of the substrate temperature and arsenic pressure. This includes both discrete RHEED intensity representation via an adaptive grid based cubic spline fitting (i.e. system identification) and the mapping of the current and reference response surfaces into each other (i.e. system optimization) (see publications 19 and 31).

2. Use of Ga^+ implanted Si_xN_y as a negative resist for UHV patterning of Si_xN_y and pattern transfer to underlying GaAs upon which MBE growth controlled nanostructures are created (see publication 7).

II.4. Nanoscale Buried Structures and Overlayer-on-Mesa Stress Simulations:

1. Utilizing molecular dynamics simulations of the Ge/Si system as a vehicle, found that the growth – controlled pyramidal three-dimensional island nanostructures formed during strained epitaxy, when buried by an appropriate overlayer, give rise to a stress at the overlayer surface that varies inversely with the distance from the island center and scales essentially with the surface area of the island. This is in stark contrast to the inverse cubic distance dependence, and scaling with the buried object volume, found for spherical objects, the model that is most commonly employed to examine the nature and consequences of buried nanostructure (i.e. quantum dot) stress and strain (see publication 55).

2. Developed and validated inter-atomic potentials for GaAs, AlAs, InAs, and their pseudo-binary alloys to enable meaningful molecular dynamics simulations of nanostructures made of these technologically important semiconductors.

3. Performed multi-million atom molecular dynamics simulations to examine strain relaxation in InAs overlayers on GaAs(001) square mesas to shed light on the self-limiting growth we found experimentally. As a function of overlayer thickness, the in-plane lattice constant of InAs parallel to the InAs/GaAs(001) interface is found to begin to exceed that of the InAs bulk value at 12 monolayers (ML). The corresponding hydrostatic stress in the overlayer revealed a change from compressive to tensile. This is consistent with our experimentally observed self-limiting InAs overlayer thickness of~12ML for mesa linear dimensions ~100nm (see publications 54 and 56).

III. Personnel:

The list of senior researchers comprises the PI, Co-PIs, and senior postdocs as noted below:

A. Madhukar (PI)

P. Chen (Co-PI)

R. K. Kalia (Co-PI)

I. G. Rosen (Co-PI)

C. Wang (Co-PI)

R. Viswanathan

M. E. Bachlechner

Under this MURI, 10 Ph.D. and seven Master's degree students were fully or partially supported (the last graduate student who got started with MURI support is to graduate in Aug.2002). Additionally, 6 post doctoral fellows were supported. Of the Ph.D.'s graduated, 4 are now working in semiconductor manufacturing R&D at Intel, Motorola, Conexant; 4 in modeling/high performance computing, and 1 in finance industry. Of the MS graduates, 6 are working in industry and one continuing with PhD. Of the 6 Post Docs, 3 are in industry, 2 in faculty positions, and 1 in a government laboratory.

IV. List of Publications:

1. Tsuruta, A. Omeltchenko, R. K. Kalia, and P. Vashishta, "Early stages of sintering of silicon nitride nanoclusters: a molecular dynamics study on parallel machines," in MRS Proc. **408**, 181 (1996).

2. M. E. Bachlechner, I. Ebbsjö, R. K. Kalia, and P. Vashishta, "Molecular-dynamics study of Si/Si_3N_4 interface," in Mat. Res. Soc. **446**, 157 (1996).

3. T. J. Campbell, A. Nakano, A. Omeltchenko, R. K. Kalia, and P. Vashishta, "Fracture in silicon nitride and alumina thin films: a molecular dynamics study," in MRS Proc. **446**, 163 (1996).

4. A. Nakano, R. K. Kalia, and P. Vashishta, "Dynamics and morphology of cracks in silicon nitride films: a molecular-dynamics study on parallel computers," in MRS Proc. **408**, 205 (1996).

5. P. Vashishta, , R. K. Kalia, W. Li, A. Nakano, A. Omeltchenko, K. Tsuruta, J. Wang, and I. Ebbsjö, "Million atom molecular-dynamics simulation on parallel computers," Current Opinion, Solid State and Materials Science **1**, 853 (1996).

6. W. Yu and A. Madhukar, "A molecular dynamics study of coherent island energetics, stresses, and strains in highly strained epitaxy," Phys. Rev. Lett. **79**, 905 (1997).

7. A. Kalburge, A. Konkar, T. R. Ramachandran, P. Chen, and A. Madhukar, "Focused ion beam assisted chemically etched mesas on GaAs(001) and the nature of subsequent molecular beam epitaxial growth," J. Appl. Phys. **82**, 859 (1997).

8. G. L. Zhao and M. E. Bachlechner, "Electronic structure, charge distribution, and charge transfer in α- and β-Si_3N_4 and at the $Si(111)/Si_3N_4(001)$ interface," Europhys. Lett. **37**, 287 (1997).

9. R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, and P. Vashishta, "Role of ultrafine microstructures in dynamic fracture in nanophase silicon nitride," Phys. Rev. Lett. **78**, 2144 (1997).

10. A. Omeltchenko, J. Yu, R. K. Kalia, and P. Vashishta, "Crack propagation and fracture in a graphite sheet: a molecular-dynamics simulation on parallel computers," Phys. Rev. Lett. **78**, 2148 (1997).

11. R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, and P. Vashishta, "Million atom molecular dynamics simulation of nanophase silicon nitride," in Symp. Proc. of Minerals, Metals & Materials Society Meeting, 89 (1997).

12. K. Tsuruta, A. Omeltchenko, A. Nakano, R. K. Kalia, and P. Vashishta, "Structure, mechanical properties, and dynamic fracture in nanophase silicon nitride via parallel molecular dynamics," in MRS Proc. **457**, 205 (1997).

13. A. Nakano, R. K. Kalia, and P. Vashishta, "Fracture of nanophase ceramics: a molecular-dynamics study," in MRS Proc. **457**, 187 (1997).

14. G. L. Zhao and M. E. Bachlechner, "Electronic structure, charge distribution, and charge transfer in α- and β-Si_3N_4 and at the $Si(111)/Si_3N_4(001)$ interface," Europhys. Lett. **37**, 287 (1997).

15. A. Nakano, T. Campbell, R. K. Kalia, and P. Vashishta, "Multilevel algorithms for computational high-temperature materials research," in Computer-aided Design of High-temperature Materials, edited by R. K. Kalia, A. Pechenik, and P. Vashishta, Oxford Univ. Press, 422 (1997).

16. A. Omeltchenko, K. Tsuruta, A. Nakano, R. K. Kalia, P. Vashishta, O. Shenderova, and D. W. Brenner, "Dynamic fracture in nanophase ceramics and diamond films: multimillion atom parallel molecular-dynamics simulations," in Computer-aided Design of High-temperature Materials, edited by R. K. Kalia, A. Pechenik, and P. Vashishta, Oxford Univ. Press, 81 (1997).

17. K. Tsuruta, J. Wang, A. Nakano, A. Omeltchenko, R. K. Kalia, and P. Vashishta, "Structure and dynamics of consolidation and fracture of nanophase ceramics via parallel molecular dynamics," in Computer-aided Design of High-temperature Materials, edited by R. K. Kalia, A. Pechenik, and P. Vashishta, Oxford Univ. Press, 323 (1997).

18. A. Nakano, R. K. Kalia, H. Kikuchi, S. Kodiyalam, K. Tsuruta, and P. Vashishta, "Fracture and microstructures of gallium arsenide: a large-scale molecular dynamics study," in MRS Spring '98 Abstracts **BB7.5**, 438 (1998).

19. P. Chen, C. Wang, A. Madhukar, T. Khan, A. Small, Z. Yan, and R. Viswanathan, "Reflection high-energy electron diffraction as an intrinsic material property sensor for machine condition transfer function in molecular beam epitaxial growth of III-V compound semiconductors," MRS Proceedings **502**, 47 (1998).

20. G. L. Zhao and M. E. Bachlechner, "Electronic structure and charge transfer in α- and β-Si_3N_4 and at the $Si(111)/Si_3N_4(001)$ interface using LCAO," Phys. Rev. B **58** (4), 1887 (1998).

21. I. G. Rosen, T. Parent, P. Chen, C. Wang, R. Heitz, M. Nagarajan, and A. Madhukar, "Feedback control of thermal chlorine (Cl_2) etching of gallium arsenide (GaAs) using in-situ spectroscopic ellipsometry sensing," Proc. of The American Control Conference, June 24-26, 1998, Philadelphia, PA, pp. 2150-2154 (1998).

22. K. Tsuruta, A. Nakano, R. K. Kalia, and P. Vashishta, "Dynamics of consolidation and crack growth in nanocluster-assembled amorphous silicon nitride," J. Am. Ceram. Soc. **81**, 433 (1998).

23. M. E. Bachlechner, A. Omeltchenko, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, A. Madhukar, and P. Messina, "Multimillion-atom molecular dynamics simulation of atomic level stresses in $Si(111)/Si_3N_4(0001)$ nanopixels," Appl. Phys. Lett. **72**, 1969 (1998).

24. T. Parent, R. Heitz, P. Chen, and A. Madhukar, "Real-time feedback control of thermal Cl_2 etching of GaAs based on in-situ spectroscopic ellipsometry," Mat. Res. Soc. Symp. Proc. **502**, 71 (1998).

25. P. Vashishta, M. E. Bachlechner, R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, I. Ebbsjö, and A. Madhukar, "Multimillion atom molecular dynamics simulations of ceramic materials and interfaces on parallel computers," in Proceedings of the Special Symposium on Advanced Materials, edited by T. Imura, H. Fujita, T. Ichinokawa, and H. Kawazoe, Nagoya, Japan, 47 (1998).

26. A. Nakano, M. E. Bachlechner, T. J. Campbell, R. K. Kalia, A. Omeltchenko, K. Tsuruta, P. Vashishta, S. Ogata, I. Ebbsjö, and A. Madhukar, "Atomistic simulation of nanostructured materials using parallel multiresolution algorithms," IEEE Computational Science & Engineering **5** (4), 68 (1998).

27. A. Nakano, R. K. Kalia, and P. Vashishta, "Multilevel algorithms for large-scope molecular dynamics simulations of nanostructures on parallel computers," VLSI Design **8** (1-4), 123 (1998).

28. A. Omeltchenko, A. Nakano, K. Tsuruta, R. K. Kalia, and P. Vashishta, "Structure and mechanical failure in nanophase silicon nitride: large-scale molecular-dynamics simulations on parallel computers," in Advances in Metal and Semiconductor Clusters Vol. IV: Cluster Materials, edited by M. Duncan, JAI Press, Stamford, CN, 263 (1998).

29. K. Tsuruta, A. Nakano, R. K. Kalia, and P. Vashishta, "Dynamics of consolidation and crack growth in nanocluster-assembled amorphous silicon nitride," J. of the Am. Ceram. Soc. **81**, 433 (1998).

30. T. Parent, J. Tie, and A. Madhukar, "In-situ spectroscopic ellipsometry and optical emission studies of CF_4/O_2 plasma etching of silicon nitride," Mat. Res. Soc. Symp. Proc., *In Situ Diagnostics and Modelling*, Eds. O. Auciello, A. R. Krauss, E. A. Irene, and J. A. Schultz, Materials Research Society **569**, 89 (1999).

31. C. Wang, P. Chen, A. Madhukar, and T. Khan, "A machine condition transfer function approach to run-to-run and machine-to-machine reproducibility of III-V compound semiconductor molecular beam epitaxial growth," IEEE Trans. on Semiconductor Manufacturing **12**, 66 (1999).

32. I. G. Rosen, T. Parent, C. Cooper, P. Chen, and A. Madhukar, "Locating sensitivity minimizing process inputs in the plasma enhanced chemical vapor deposition (PECVD) of silicon nitride thin films: a neural network based approach," Proc. of the 18th American Control Conf., San Diego, CA, June 2-4, 1999, pp. 3594-3599 (1999).

33. P. Walsh, A. Omeltchenko, H. Kikuchi, R. K. Kalia, A. Nakano, and P. Vashishta, "Molecular dynamics simulations of nanoindentation of silicon nitride," Mat. Res. Soc. Symp. Proc. **539**, 119 (1999).

34. S. Kodiyalam, A. Chatterjee, I. Ebbsjö, R. K. Kalia, H. Kikuchi, A. Nakano, J. P. Rino, and P. Vashishta, "Pressure induced structural transformation in nanocluster assembled gallium arsenide," Mat. Res. Soc. Symp. Proc. **536**, 545 (1999).

35. A. Nakano, T. Campbell, R. K. Kalia, and P. Vashishta, "Multilevel algorithms for computational high-temperature materials research," in Computer-aided Design of High-temperature Materials, edited by A. Pechenik, R. K. Kalia, and P. Vashishta, Oxford Univ. Press, Oxford, 422 (1999).

36. M. E. Bachlechner, A. Omeltchenko, K. Tsuruta, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, and A. Madhukar, "Structural correlations and stress distribution at silicon/silicon nitride interface," in Computer-Aided Design of High-Temperature Materials, edited by A. Pechenik, R. K. Kalia, and P. Vashishta, Oxford Univ. Press, Oxford, 244 (1999).

37. I. G. Rosen, T. Parent, R. Mancera, P. Chen, and A. Madhukar, "Modelling and validation of sensor and actuator dynamics for, and real time feedback control of, thermal chlorine etching of gallium arsenide," Proceedings of 1999 Spring Meeting of the Materials Research Society (MRS) Symposium U, April 5-9, 1999, San Francisco, CA, *In-situ Process Diagnostics and Modelling*, Eds. O. Auciello, A. R. Krauss, E. A. Irene, and J. A. Schultz, Materials Research Society **569**, 159 (1999).

38. M. E. Bachlechner, R. K. Kalia, A. Nakano, A. Omeltchenko, P. Vashishta, I. Ebbsjö, A. Madhukar, and G.-L. Zhao, "Structural correlations at Si/Si_3N_4 interface and atomic stress in Si/Si_3N_4 nanopixels--10 million-atom molecular dynamics simulation on parallel computers," Journal of the European Ceramic Society **19**, 2265 (1999).

39. A. Chatterjee, T. Campbell, R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, and P. Vashishta, "Parallel molecular dynamics simulations of high temperature ceramics," Journal of the European Ceramic Society **19**, 2257 (1999).

40. A. Nakano, R. K. Kalia, and P. Vashishta, "Scalable molecular-dynamics, visualization, and data-management algorithms for materials simulations," Computing in Science & Engineering **1** (5), 39 (1999).

41. P. Vashishta, R. K. Kalia, and A. Nakano, "Large-scale atomistic simulation of dynamic fracture," Computing in Science & Engineering **1** (5), 56 (1999).

42. M. E. Bachlechner, A. Omeltchenko, P. Walsh, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjo, and A. Madhukar, "Molecular dynamics study of Si/Si_3N_4 interface and $Si/Si/Si_3N_4$ mesa," in Proceedings of MRS Symposium **592**, 369 (2000).

43. X. Su, R. K. Kalia, A. Madhukar, A. Nakano, and P. Vashishta, "Multimillion atom simulation of atomic-level surface stresses on InAs/GaAs nanomesas," Proc. of MRS Symposium, Fall 1999, **548**, 269 (2000).

44. I. G. Rosen, T. Parent, B. Fidan, and A. Madhukar, "In-situ spectroscopic ellipsometry for the real-time process control of plasma etching of silicon," Proceedings of 1999 Fall Meeting of Materials Research Society (MRS) Symposium S, Nov 29-Dec 3, 1999, Boston, MA, in

Non Destructive Methods for Materials Characterization, edited by T. Matikas, N. Meyendorf, G. Baaklini and R. Gilmore, Materials Research Society **591**, 263 (2000).

45. B. Fidan, I. G. Rosen, T. Parent, and A. Madhukar, "Spectroscopic ellipsometry based real-time control of CF_4/O_2 plasma etching of silicon nitride," in Proc. of 2000 American Control Conf., June 28-30, 2000, Chicago, IL, pp. 4006-4010 (2000).

46. A. Omeltchenko, M. E. Bachlechner, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, A. Madhukar, and P. Messina, "Stress domains in $Si(111)/Si_3N_4(0001)$ nanopixel - 10 million-atom molecular dynamics simulations on parallel computers," Physical Review Letters **84**, 318 (2000).

47. M. E. Bachlechner, A. Omeltchenko, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, and A. Madhukar, "Dislocation emission at silicon/silicon nitride interface - a million atom molecular dynamics simulation on parallel computers," Physical Review Letters **84**, 322 (2000).

48. I. Ebbsjö, R. K. Kalia, A. Nakano, J. P. Rino, and P. Vashishta, "Topology of amorphous gallium arsenide on intermediate length scales: a molecular dynamics study," Journal of Applied Physics **87**, 7708 (2000).

49. R. K. Kalia, T. J. Campbell, A. Chatterjee, A. Nakano, P. Vashishta, and S. Ogata, "Multiresolution algorithms for massively parallel molecular dynamics simulations of nanostructured materials," Computer Physics Communications **128**, 245 (2000).

50. A. Omeltchenko, T. J. Campbell, R. K. Kalia, X. Liu, A. Nakano, and P. Vashishta, "Scalable I/O of large-scale molecular-dynamics simulations: a data-compression algorithm," Computer Physics Communications **131**, 78 (2000).

51. P. Vashishta, M. E. Bachlechner, T. J. Campbell, R. K. Kalia, H. Kikuchi, S. Kodiyalam, A. Nakano, S. Ogata, F. Shimojo, and P. Walsh, "Multimillion atom simulations of nanostructured materials on parallel computers - sintering and consolidation, fracture, and oxidation," Progress of Theoretical Physics Supplement **138**, 175 (2000).

52. I. G. Rosen, T. Parent, C. Cooper, P. Chen, and A. Madhukar, "A neural network based approach to determining a robust process recipe for the plasma enhanced deposition of silicon nitride thin films," IEEE Transactions on Control Systems Technology **9**, 271 (2001).

53. B. Fidan, I. G. Rosen, T. Parent, J. Tie, and A. Madhukar, "Multivariable intelligent control of CF_4/O_2 plasma etching of silicon nitride," Proceedings of 2001 American Control Conference, Arlington, VA, July 25-27, **2**, 1280 (2001).

54. X. Su, R. K. Kalia, A. Nakano, P. Vashishta, and A. Madhukar, "Million-atom molecular dynamics simulation of flat InAs overlayers with self-limiting thickness on GaAs square nanomesas," Appl. Phys. Lett. **78**, 3717 (2001).

55. M. A. Makeev and A. Madhukar, "Simulations of atomic level stresses in systems of buried Ge/Si islands," Phys. Rev. Lett. **86**, 5542 (2001).

56. X. Su, R. K. Kalia, A. Nakano, P. Vashishta, and A. Madhukar, "Critical lateral size for stress domain formation in InAs/GaAs square nanomesas: a multimillion-atom molecular dynamics study," Appl. Phys. Lett. **79**, 4577 (2001).

57. I. G. Rosen, T. Parent, B. Fidan, C. Wang, and A. Madhukar, "Design, development and testing of real-time feedback controllers for semiconductor etching processes using in-situ spectroscopic ellipsometry sensing," IEEE T. Contr. Syst. T. **10** (1), 64 (2002).

58. I. G. Rosen, T. Parent, P. Chen, R. Mancera, and A. Madhukar, "Modeling and simulation of thermal chlorine etching of gallium arsenide with application to real time feedback control," Math. Comput. Model. **35** (3-4), 335 (2002).

59. I. G. Rosen, T. Parent, C. Wang and A. Madhukar, "An elementary model for a semiconductor etching process," SIAM Review, (Submitted).

V. Interactions / Transitions

(a). Participation/Presentations at Conferences, Seminars, etc.

Between the PI, Co-PIs, and postdocs, this MURI team made over 50 invited presentations at various national and international conferences and academic, industrial, and government laboratories. Additionally, over 20 contributed presentations at conferences were made.

(b) External Interactions / Knowledge Transfer

The most important transition of knowledge / research results has been in the form of the trained Ph.D. students and postdocs hired by the semiconductor industry (see numbers below). Specifically, Tyler Parent, who did his Ph.D. on spectroscopic ellipsometry based adaptive real time control of plasma etching, was hired by Intel where he continues to push the frontiers of etching; likewise, Amol Kalburge, who did his Ph.D. on in-situ focused ion beam assisted patterning and subsequent growth controlled nanostructure formation joined Conexant where he is in charge of developing the front end etching processes; as a third example, Timothy Campbell, who did his Ph.D. on the massively parallel molecular dynamics simulations is now working at NAVO, a DoD_MSRC high performance computing site in Mississippi.

Additionally, external interactions occurred with the following:

1. Motorola, with Ceramics Division in Phoenix, Arizona.

2. Argonne National Laboratory, concerning neutron scattering and MD studies of silicon nitride.

3. LSI Logic, Inc. concerning plasma process real time monitoring and control.

4. Intel Corp., concerning plasma process modeling, monitoring, and control.

5. Air Force Wright-Patterson Lab., concerning scalable parallel molecular dynamics and in-situ monitoring of MBE growth.

6. Air Force Philips Lab., concerning molecular dynamics simulations.

Amongst the postdocs trained, Ravi Viswanathan was lured away by then Rockwell (now Conexant) where he has been leading one of the semiconductor processing groups, and another postdoc, Rajesh Krishnamurthy, was hired away by Nortel, also for his expertise in semiconductor processing acquired as part of this MURI efforts.

VI. Honors/Recognition:

- DARPA Sustained Excellence Performer Award, USC-LSU MURI Team, Ultra Electronics Program, 1997.